

REPORT DOCUMENTATION PAGE

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1. REPORT DATE (DD-MM-YYYY)

2. REPORT TYPE
Technical Papers

3. DATES COVERED (From - To)

4. TITLE AND SUBTITLE

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

5d. PROJECT NUMBER

2303

5e. TASK NUMBER

m2c8

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory (AFMC)
AFRL/PRS
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8. PERFORMING ORGANIZATION
REPORT

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

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10. SPONSOR/MONITOR'S
ACRONYM(S)

11. SPONSOR/MONITOR'S
NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

1121 012

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:

a. REPORT

Unclassified

b. ABSTRACT

Unclassified

c. THIS PAGE

Unclassified

17. LIMITATION
OF ABSTRACT

A

18. NUMBER
OF PAGES

19a. NAME OF RESPONSIBLE
PERSON

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19b. TELEPHONE NUMBER

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Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39.18

62

separate items are enclosed

C8

MEMORANDUM FOR PRS (Contractor/In-House Publication)

FROM: PROI (TI) (STINFO)

26 September 2000

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2000-181**
Christe, K.O. (ERC); Vij, Ashwani; Mews, R.; Zhang, X. (USC), Boatz, J. (PRSP), "Method for Solving
Some Disordered Crystal Structures and its Application to the Structures of NF₂O+ and SO₂F-"
(Oral Presentation)

15th Winter Fluorine Conference (St. Petersburg, FL, 14 Jan 2001)
(Past Deadline: 14 Sep 2000)

(Statement A)

1. This request has been reviewed by the Foreign Disclosure Office for: a.) appropriateness of distribution statement,
b.) military/national critical technology, c.) export controls or distribution restrictions,
d.) appropriateness for release to a foreign nation, and e.) technical sensitivity and/or economic sensitivity.

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2. This request has been reviewed by the Public Affairs Office for: a.) appropriateness for public release
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appropriateness of distribution statement, d.) technical sensitivity and economic sensitivity, e.) military/
national critical technology, and f.) data rights and patentability

Comments: _____

APPROVED/APPROVED AS AMENDED/DISAPPROVED

PHILIP A. KESSEL
Technical Advisor

Date

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METHOD FOR SOLVING SOME DISORDERED CRYSTAL STRUCTURES AND ITS APPLICATION TO THE STRUCTURES OF NF_2O^+ AND SO_2F^- . **Karl O. Christe**, Ashwani Vij, Rudiger Mews, Xiongzhi Zhang, Jerry Boatz., Air Force Research Laboratory, Edwards AFB, CA 93524 and University of Southern California, Los Angeles, CA 90089, University of Bremen, Bremen, Germany.

Oxygen and fluorine ligands are similar in size and frequently exhibit positional disorder in the crystal structures of oxofluorides, resulting in a partial or complete averaging of the observed bond lengths and angles. The failure to recognize the presence of disorder has resulted in the publication of numerous incorrect structures, while the recognition of disorder problems has generally prompted researchers to abandon these data sets. In this paper, a method is outlined which allows in favorable cases the extraction of the correct individual bond lengths and angles from disordered data. The method is demonstrated for the SO_2F^- and NOF_2^+ ions, and the correctness of the derived bond lengths is supported by ab initio calculations for the free ions.

ABSTRACT. Please be BRIEF—150 words maximum if possible. Title of paper should be ALL CAPS; author(s) listed by first name, middle initial, last name; indicate address with zip code.

A. DIVISION OF FLUO Division Member ☒ Yes ☐ No

B. ACS MEMBER ☒ Yes ☐ No

C. TITLE OF PAPER Method for solving some disordered crystal structures and its application to the structures of NF_2O^+ and SO_2F^-

Please indicate preference: ☒ Oral ☐ Poster
☐ withdraw if oral/poster format cannot be met

D. AUTHORS

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First Name

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(To be filled in by Division)

Paper number as listed on program _____

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G. For contributed papers, do authors
meet criteria outline in ACS Bylaw VI,
Section 6(3)? See instructions.

☐ Yes ☐ No

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Equipment

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